Connecting via Winsock to STN

Welcome to STN International! Enter x:x

FILE 'HOME' ENTERED AT 11:07:07 ON 11 JUN 2007

=> file reg

=>

Uploading C:\Program Files\Stnexp\Queries\10519208.str

chain nodes :
21 22 24 25 27 28 29 30 31 32 35 37 39
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
chain bonds :
1-32 2-31 3-30 6-37 7-21 8-39 9-19 13-24 14-25 15-27 16-28 17-35 18-29

ring bonds:
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 11-12 11-16 11-17 12-13 12-20 13-14 14-15 15-16 17-18 18-19 19-20 exact/norm bonds:
1-32 2-31 3-30 6-37 7-21 11-17 12-20 13-24 14-25 15-27 16-28 17-18 17-35 18-19 18-29 19-20 20-22 exact bonds:
4-7 5-10 7-8 8-9 8-39 9-10 9-19 normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 isolated ring systems: containing 1:11:

G1:C,H,O

G2:H,Cb,Cy,Hy

G3:C,H,O,Cb,Cy,Hy

#### Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 22:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 35:CLASS 37:CLASS 39:CLASS

#### L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR

G1 C,H,O

G2 H,Cb,Cy,Hy

G3 C, H, O, Cb, Cy, Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

L3 21 SEA SSS FUL L1

=> file ca

=> s 13

L4 1 L3

=> d ibib abs fhitstr

L4 ANSWER 1 OF 1 CA COPYRIGHT 2007 ACS ON STN
ACCESSION NUMBER: 140:59525 CA
TITLE: Preparation of
3-(4-0x0-4H-chromen-2-yl)-(1H)-quinolin4-ones 88 anticancer agents
Frion, Jean Daniel, Israel, Lucien, Le Ridant, Alain,
Harpey, Catheriner, Rabhi, Cherif, Bl Kaloun, Bachir
PATENT ASSIGNEE(S): Les Laboratoires Servier, Fr.; Servier Lab
SOURCE: PRXXBL
DOCUMENT TYPE: Persent DOCUMENT TYPE: LANGUAGE: PAMILY ACC. NUM. COUNT: PATENT INFORMATION: APPLICATION NO PATENT NO. KIND DATE DATE WO 2003-FR1849 MARPAT 140:59525 OTHER SOURCE(S):

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

ANSWER 1 OF 1 CA COPYRIGHT 2007 ACS on STN (Continued)
Title compds. I [wherein R1, R2, R3, R4, R6, R8, R9, R10 = H, OH, alkyl,
aryl/alkoxy,arbonyl/alkoxy, arylalkoxy, and alkoxycarbonylalkoxy, R5 =
alkyl, (un)substituted hetero/aryl, R7 = H, OH, alkoxy, cyclo/alkyl, or

- (un)substituted nitrogen or oxygen heterocycle, their optical isomers, pharmaceutical acceptable salts with acids, hydrates and solvates) were prepared as anticancer agents. For example, IT was prepare by

of 2,4-dimethoxy-6-hydroxyacetophenone (preparation given) with

2-acetyl-5-methoxyphenyl-4-oxo-1-phenyl-1, 4-dihydroquinoline-1-carboxylate (preparation given), rearrangement in the presence of BuOK/DMF/THF, cyclization
in the presence of AcOH/H2SO4, and deprotection. In an in vitro cytotoxicity test, II showed an IC50 ranging from 0.25 µM to 0.05 µM towards five tumor cell lines. I exhibited a synergistic effect with several well-known anticancer agents (no data). Selected I induced apoptosis in 8 h.

IT 637362-92-6P, 3-(7-Methoxy-4-oxo-4H-1-benzopyran-2-yl)-1-phenyl-1,4-dihydroquinolin-4-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USBS (Uses)
(anticancer agent; preparation of oxochromenylquinolinones as anticancer

anticancer agent, preparation of oxochromenyiquinolinones as anticancer agents |
RN 637362-92-6 CA | CN 4(1H)-Quinolinone, 3-(7-methoxy-4-oxo-4H-1-benzopyran-2-y1)-1-phenyl-(9CI) (CA INDEX NAME)

THERE ARE 2 CITED REPERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

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10/519,208
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=> file marpat

Expanded G-group definition display now available.

=> s l1 full

L5 1 SEA SSS FUL L1

=> d ibib abs fqhit

L5 ANSMER 1 OF 1 MARPAT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 140:59525 MARPAT
TITLE: 170:59525 MARPAT
TITLE: 4-ones as anticancer agents

INVENTOR(9): Brion, Jean Daniel, Israel, Lucien, Le Ridant, Alain,
Harpey, Catherine; Rabhi, Cherif, El Kaloun, Bachir

Les Laboratoires Servier, Fr.; Servier Lab

COURENT TYPE: Patent

LANGUAGE: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: FRXBL

DAMILLY ACC. NUM. COUNT: 1

PAMELLY ACC. NUM. COUNT: 1

PAMELLY ACC. NUM. COUNT: 1

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

						KIND DATE			APPLICATION NO.										
		2841														0619			
		2841																	
										CA 2003-2489136				20030618					
										WO 2003-FR1849									
															BZ,			CN.	
															GB,				
															KZ,				
															NO.				
															TN.				
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		DW.											UG	2M	ZW,	MA	A.Z	BY	
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															NE,				
	AU	2003																••	
					A1 2005					EP 2003-750780									
										GB.	GR.	IT.	LI.	LU.	NL.	SE.	MC.	PT.	
															EE.				
	BR	2003																	
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	AT	3236	98		т		2006	0515		A.	T 20	03-7	5078	0	2003	0618			
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	NO	2004	0055	40	А		2004	1217		N	0 20	04-5	540		2004	1217			
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GΙ																			

STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Title compds. I (wherein R1, R2, R3, R4, R6, R8, R9, R10 = H, OH, alkyl, aryl/alkoxycarbonyl/alkoxy, arylalkoxy, and alkoxycarbonylalkoxy, R5 = alkyl, (un)substituted hetero/aryl; R7 = H, OH, alkoxy, cyclo/alkyl, or

ANSWER 1 OF 1 MARPAT COPYRIGHT 2007 ACS on STN (Continued)

L5 ANSWER 1 OF 1 MARPAT COPYRIGHT 2007 ACS on STN (Continued) = (un)substituted nitrogen or oxygen heterocycle, their optical isomers, pharmaceutical acceptable salts with acids, hydrates and solvates) were prepd. as anticancer agents. For example, II was prep. by esterification of 2,4-dimethoxy-6-hydroxyacetophenone (prepn. given) with

2-acetyl-5-methoxyphenyl-4-oxo-1-phenyl-1,4-dihydroquinoline-3-carboxylate (prepn. given), rearrangement in the presence of BuOK/DMF/THF, cyclization
in the presence of AcOH/H2SO4, and deprotection. In an in vitro cytotoxicity test, II showed an ICSO ranging from 0.25 µM to 0.05 µM towards five tumor cell lines. I exhibited a synergistic effect with several well-known anticancer agents (no data). Selected I induced apoptosis in 8 h.

MSTR 1

= alkyl <containing 1-6 C>
= carbocycle <containing 6-10 C, aromatic,
6 or more normalized bonds, mono- or bicyclic,
(1-2) 6-membered rings only> (opt. substd. by 1 or more G3)
= alkyl <containing 1-6 C>
= 9

Patent location: Note: claim 1
and pharmaceutically acceptable acid addition
salts, hydrates, and solvates
also incorporates claim 10, formulas IV, V, VII,
and VIII
additional ring formation also claimed
optical isomers

Note:

Note: Stereochemistry:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE REFERENCE COUNT:

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10/519,208
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## => file reg

=>

Uploading C:\Program Files\Stnexp\Queries\11519208.str

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chain nodes :
21 22
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
7-21 9-19 20-22
ring bonds :
            3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 11-12 11-16 11-17 12-13
1-2 1-6 2-3
12-20 13-14 14-15 15-16 17-18 18-19 19-20
exact/norm bonds :
7-21 11-17 12-20 17-18 18-19 19-20 20-22
exact bonds :
4-7 5-10 7-8 8-9 9-10 9-19
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16
isolated ring systems :
containing 1 : 11 :
```

G1:C,H,O

G2:H,Cb,Cy,Hy

G3:C,H,O,Cb,Cy,Hy

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 22:CLASS

## L6 STRUCTURE UPLOADED

=> d 16

L6 HAS NO ANSWERS L6 STR

G1 C,H,O

G2 H, Cb, Cy, Hy

G3 C, H, O, Cb, Cy, Hy

Structure attributes must be viewed using STN Express query preparation.

=> s 16 full

L8 . 22 SEA SSS FUL L6

=> file ca

=> s 18

L9 1 L8

=> d his

(FILE 'HOME' ENTERED AT 11:07:07 ON 11 JUN 2007)

FILE 'REGISTRY' ENTERED AT 11:07:14 ON 11 JUN 2007

L1 STRUCTURE UPLOADED

L2 1 S L1 SAM

L3 21 S L1 FULL

FILE 'CA' ENTERED AT 11:07:41 ON 11 JUN 2007

L4 1 S L3

FILE 'MARPAT' ENTERED AT 11:07:49 ON 11 JUN 2007 L5 1 S L1 FULL

FILE 'REGISTRY' ENTERED AT 11:08:05 ON 11 JUN 2007

L6 STRUCTURE UPLOADED

L7 1 S L6 SAM 22 S L6 FULL L8

FILE 'CA' ENTERED AT 11:09:02 ON 11 JUN 2007

1 S L8 L9

=> s 19 not 14

L100 L9 NOT L4

=> file reg

Uploading C:\Program Files\Stnexp\Queries\12519208.str

chain nodes :

21 22

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

chain bonds :

7-21 9-19 20-22

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 11-12 11-16 11-17 12-13

12-20 13-14 14-15 15-16 17-18 18-19 19-20

exact/norm bonds :

4-7 5-10 7-8 7-21 8-9 9-10 11-17 12-20 17-18 18-19 19-20 20-22

exact bonds :

9-19

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

G1:C,H,O

G2:H,Cb,Cy,Hy

G3:C,H,O,Cb,Cy,Hy

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 22:CLASS

# L11 STRUCTURE UPLOADED

=> d 111 L11 HAS NO ANSWERS L11 STR

G1 C, H, O

G2 H, Cb, Cy, Hy

G3 C, H, O, Cb, Cy, Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l11 full

L12 22 SEA SSS FUL L11

=> d his

(FILE 'HOME' ENTERED AT 11:07:07 ON 11 JUN 2007)

FILE 'REGISTRY' ENTERED AT 11:07:14 ON 11 JUN 2007

L1 STRUCTURE UPLOADED

L2 1 S L1 SAM L3 21 S L1 FULL

FILE 'CA' ENTERED AT 11:07:41 ON 11 JUN 2007

L4 1 S L3

FILE 'MARPAT' ENTERED AT 11:07:49 ON 11 JUN 2007 L5 1 S L1 FULL

```
FILE 'REGISTRY' ENTERED AT 11:08:05 ON 11 JUN 2007
L6
               STRUCTURE UPLOADED
L7
             1 S L6 SAM
            22 S L6 FULL
L8
    FILE 'CA' ENTERED AT 11:09:02 ON 11 JUN 2007
L9
             1 S L8
L10
             0 S L9 NOT L4
    FILE 'REGISTRY' ENTERED AT 11:09:14 ON 11 JUN 2007
L11
               STRUCTURE UPLOADED
           22 S L11 FULL
L12
=> s 112 not 13
      1 L12 NOT L3
=> s 113 full
L14
            1 L12 NOT L3
=> file ca
=> s 113
L15
            1 L13
=> s 115 not 19
L16 0 L15 NOT L9
=> file marpat
=> d his
     (FILE 'HOME' ENTERED AT 11:07:07 ON 11 JUN 2007)
     FILE 'REGISTRY' ENTERED AT 11:07:14 ON 11 JUN 2007
               STRUCTURE UPLOADED
L1
L2
             1 S L1 SAM
L3
            21 S L1 FULL
    FILE 'CA' ENTERED AT 11:07:41 ON 11 JUN 2007
      1 S L3
L4
     FILE 'MARPAT' ENTERED AT 11:07:49 ON 11 JUN 2007
            1 S L1 FULL
L_5
    FILE 'REGISTRY' ENTERED AT 11:08:05 ON 11 JUN 2007
L6
              STRUCTURE UPLOADED
L7
             1 S L6 SAM
L8
            22 S L6 FULL
    FILE 'CA' ENTERED AT 11:09:02 ON 11 JUN 2007
L9
             1 S L8
L10
             0 S L9 NOT L4
    FILE 'REGISTRY' ENTERED AT 11:09:14 ON 11 JUN 2007
              STRUCTURE UPLOADED
Lll
            22 S L11 FULL
L12
L13
            1 S L12 NOT L3
```

L14 1 S L13 FULL

FILE 'CA' ENTERED AT 11:10:24 ON 11 JUN 2007

L15 1 S L13

L16 0 S L15 NOT L9

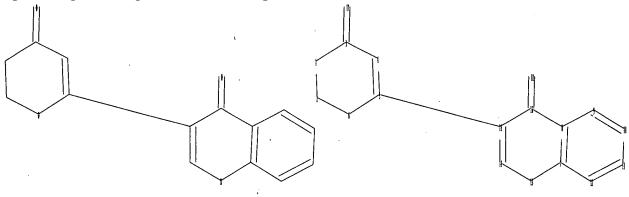
FILE 'MARPAT' ENTERED AT 11:10:43 ON 11 JUN 2007

=> s l11 full

L17 1 SEA SSS FUL L11

=> file reg

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chain nodes :
17 18
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
chain bonds :
3-17 5-15 16-18
ring bonds :
1-3 1-2 2-6 3-4 4-5 5-6 7-8 7-12 7-13 8-9 8-16 9-10 10-11 11-12 13-14
 14-15 15-16
exact/norm bonds :
1-3 1-2 2-6 3-4 3-17 4-5 5-6 7-13 8-16 13-14 14-15 15-16 16-18
exact bonds :
5-15
normalized bonds :
7-8 7-12 8-9 9-10 10-11 11-12

G1:C,H,O

G2:H,Cb,Cy,Hy

G3:C,H,O,Cb,Cy,Hy

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS

L18 STRUCTURE UPLOADED

=> d 118 L18 HAS NO ANSWERS L18 STR

G1 C, H, O

G2 H, Cb, Cy, Hy

G3 C, H, O, Cb, Cy, Hy

Structure attributes must be viewed using STN Express query preparation.

=> s l18 full

L19 22 SEA SSS FUL L18

=> d his

(FILE 'HOME' ENTERED AT 11:07:07 ON 11 JUN 2007)

FILE 'REGISTRY' ENTERED AT 11:07:14 ON 11 JUN 2007

L1 STRUCTURE UPLOADED

L2 1 S L1 SAM

L3 21 S L1 FULL

FILE 'CA' ENTERED AT 11:07:41 ON 11 JUN 2007

L4 1 S L3

FILE 'MARPAT' ENTERED AT 11:07:49 ON 11 JUN 2007

L5 1 S L1 FULL

FILE 'REGISTRY' ENTERED AT 11:08:05 ON 11 JUN 2007

STRUCTURE UPLOADED L6 Ļ7 1 S L6 SAM 22 S L6 FULL L8 FILE 'CA' ENTERED AT 11:09:02 ON 11 JUN 2007 L9 1 S L8 L10 0 S L9 NOT L4 FILE 'REGISTRY' ENTERED AT 11:09:14 ON 11 JUN 2007 L11STRUCTURE UPLOADED 22 S L11 FULL L12 L13 1 S L12 NOT L3 L14 . 1 S L13 FULL FILE 'CA' ENTERED AT 11:10:24 ON 11 JUN 2007 L15 1 S L13 L16 0 S L15 NOT L9 FILE 'MARPAT' ENTERED AT 11:10:43 ON 11 JUN 2007 1 S L11 FULL L17 FILE 'REGISTRY' ENTERED AT 11:11:07 ON 11 JUN 2007 L18 STRUCTURE UPLOADED L19 22 S L18 FULL => s 119 not 112 0 L19 NOT L12 L20 => ---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

STN INTERNATIONAL LOGOFF AT 11:12:25 ON 11 JUN 2007